

N-Cycloheptyl-N'-phenylurea
19095-79-5 | DTXSID10172606

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 7.93

Global applicability domain: Inside

Local applicability domain index: 4.31e-01

Confidence level: 5.61e-01

Nearest Neighbors from the Training Set

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N,N'-Dicyclohexylthiourea

Measured: 4.37

Predicted: 5.79

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Azacyclotridecan-2-one

Measured: 2.57

Predicted: 4.16

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Molinate

Measured: 25.7

Predicted: 14.8

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Tributylamine

Measured: 25.1

Predicted: 23.2